



chain nodes :

7 8 17 18 26 27 28 37 38 39 47 48 51 52 54 55 56 57 58 59 61 62

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 14 15 16 19 20 21 22 23 24 25 29 30 31 32 33
34 35 36 40 41 42 43 44 45 46

chain bonds :

3-8 5-7 7-59 8-58 9-11 10-19 12-17 14-18 17-61 18-62 21-29 22-28 24-27 25-26
27-57 28-56 33-39 35-38 36-37 38-54 39-55 40-41 44-48 46-47 47-51 48-52

ring bonds :

1-2 1-6 2-3 2-10 3-4 4-5 5-6 6-9 9-25 10-25 11-12 11-16 12-13 13-14 14-15 15-16
19-20 19-24 20-21 21-22 22-23 23-24 29-30 29-36 30-31 30-35 31-32 32-33 32-40
33-34 34-35 36-40 41-42 41-46 42-43 43-44 44-45 45-46

exact/norm bonds :

2-10 3-8 5-7 6-9 7-59 8-58 9-25 10-25 12-17 14-18 17-61 18-62 22-28 24-27 25-26
27-57 28-56 29-30 29-36 32-40 33-39 35-38 36-37 36-40 38-54 39-55 44-48 46-47
47-51 48-52

exact bonds :

9-11 10-19 21-29 40-41

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 19-20 19-24 20-21
21-22 22-23 23-24 30-31 30-35 31-32 32-33 33-34 34-35 41-42 41-46 42-43 43-44
44-45 45-46

G1:H,O,COOH,PO3H2,OP03H2,OSO3H,SO3H,NH,NH2,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS 28:CLASS 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:CLASS 38:CLASS 39:CLASS 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:CLASS 48:CLASS 51:CLASS 52:CLASS 54:CLASS
55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 61:CLASS 62:CLASS

